

New Statistical Techniques for Predictive Water Quality Modeling at Great Lakes Beaches



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Introduction

E. coli is used as a fecal indicator bacterium

Without rapid methods, 24 hours are required to get an answer

Environmental predictors (weather, waves, etc.) are available in real time

Our ultimate goal is to predict *E. coli* from environmental predictors.



Modeling Approaches

getting the most information from all data available

persistence model

using yesterday's *E. coli* to predict today's conditions

ordinary least squares regression (OLS)

well-established technique

requires decisions on how to handle interaction and correlation

partial least squares (PLS)

newer technique used extensively in spectroscopy

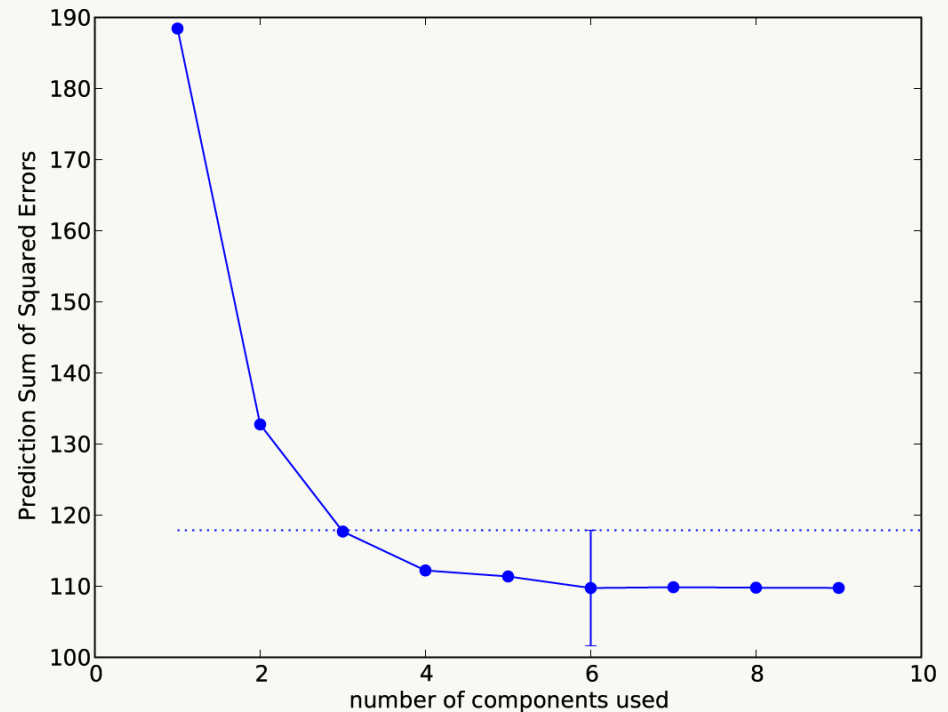
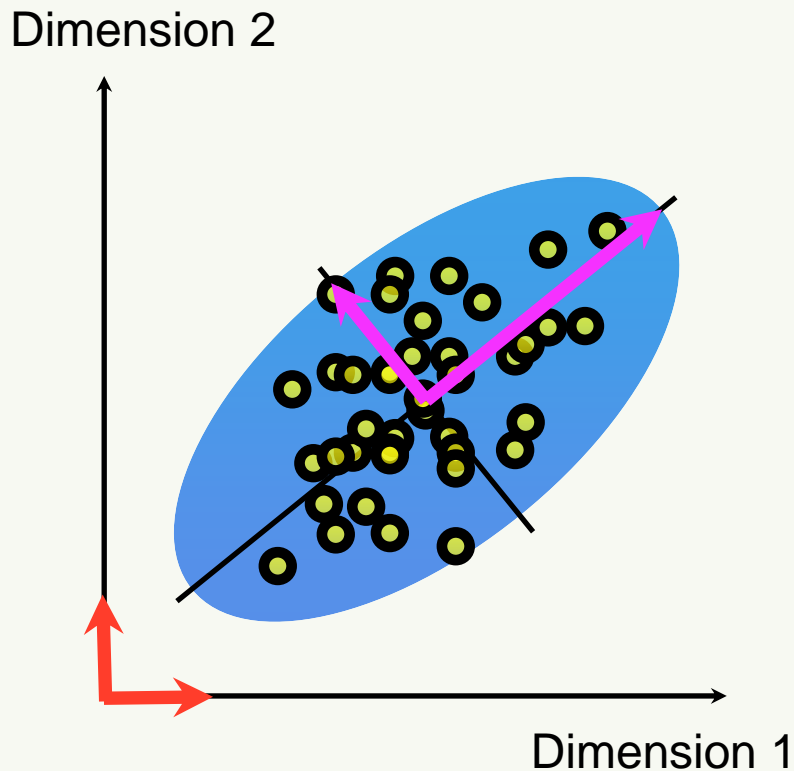
introduced to beach community by Hou, Rabinovici, and Boehm (2006)

useful when variables are correlated or insensitive

overfitting prevented through cross validation and component trimming

algorithm replaces trial-and-error interaction terms & variable selection

Partial Least Squares: Example



Partial Least Squares

regression built on principal directions relating variables to predictions

$$\mathbf{y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$$

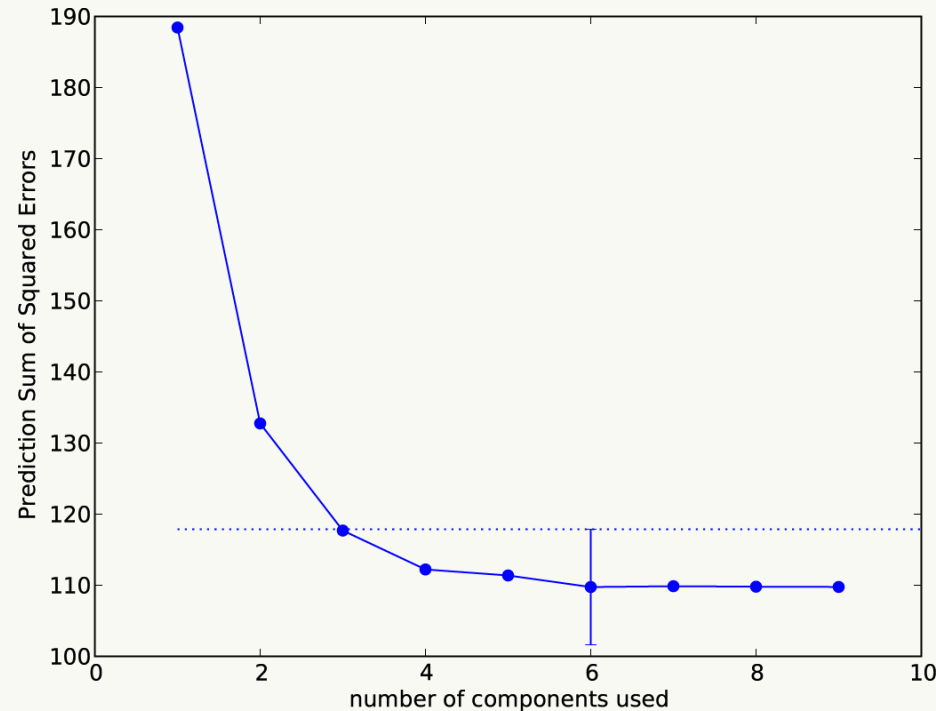
E. coli observations | predictor variables | coefficients | error term

principal directions of covariance
between \mathbf{X} and \mathbf{y} define components

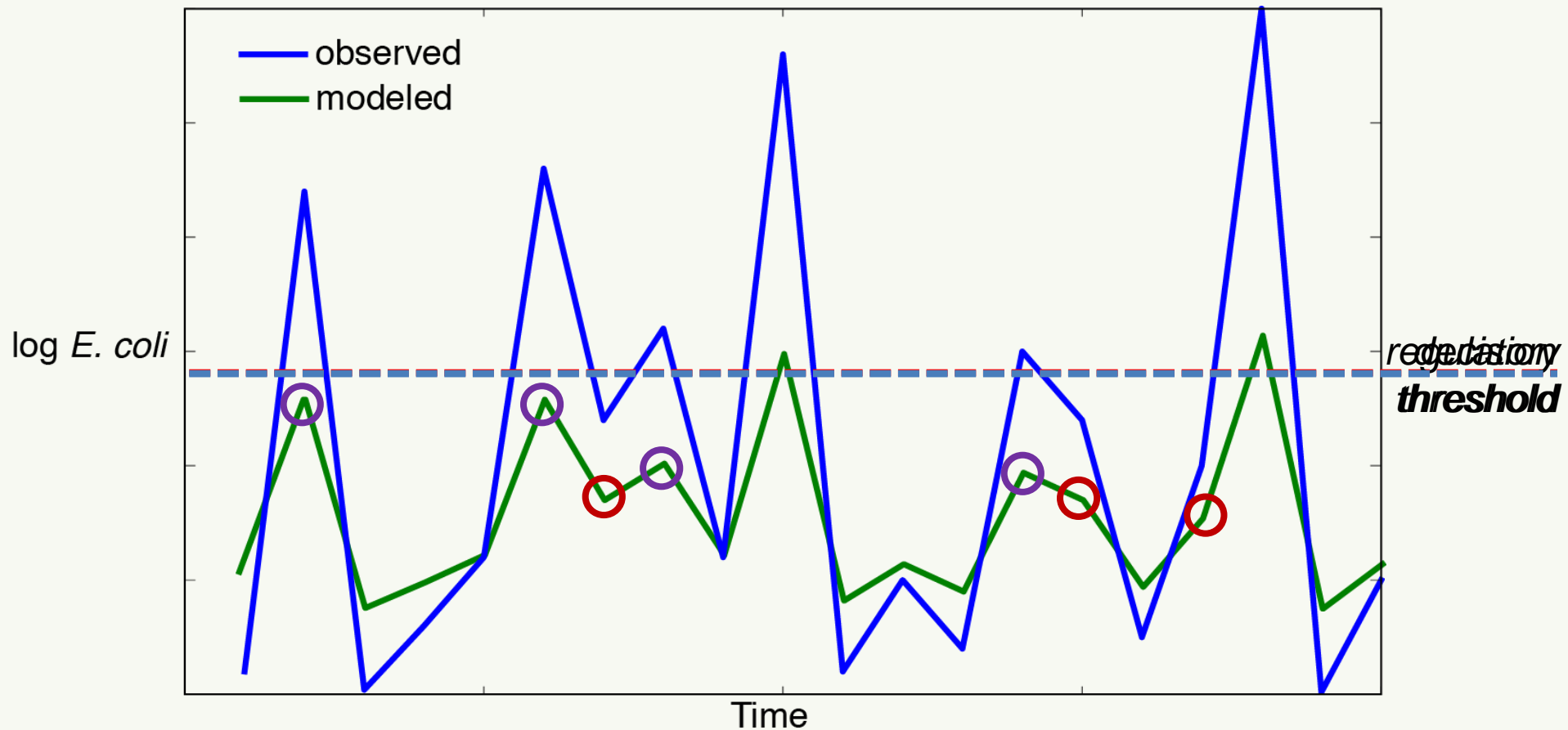
using all components is equivalent to
OLS with all variables

the number of components retained
is chosen balancing lower PRESS
against overfitting

each component includes information
from all base variables



Decision and Regulatory Thresholds

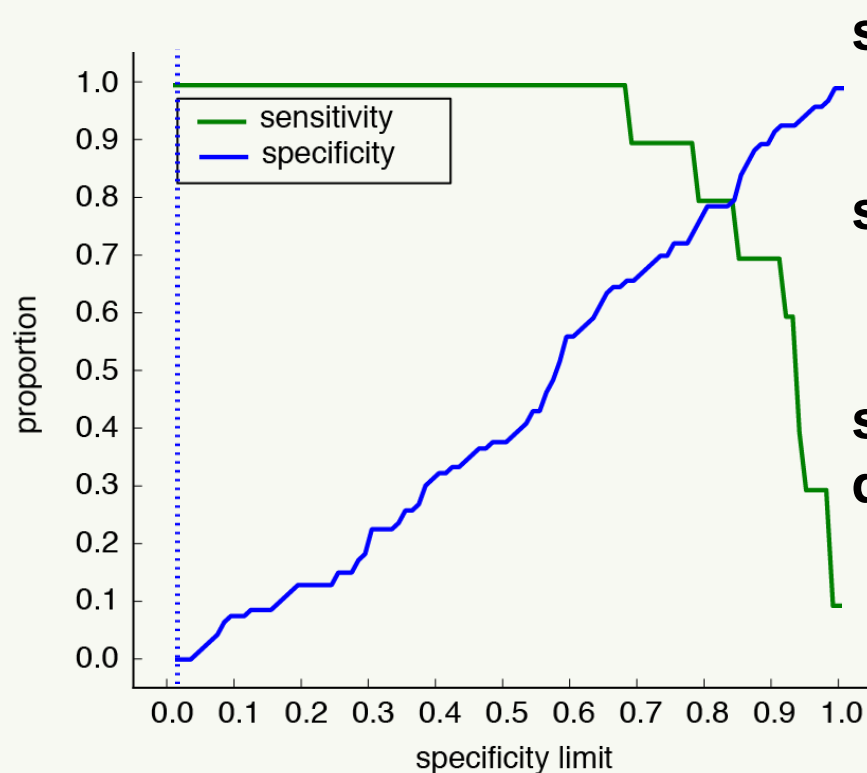


Tradeoffs for Model Performance

robust methods and improved data integration

building a PLS model

managers decide the tradeoff between protective and permissive



sensitivity: proportion of true positives
high sensitivity means increasing
true positives

specificity: proportion of true negatives
low specificity means increasing
false positives

**specificity limit (vertical blue line) is the
dial controlling this tradeoff**



Great Lakes Beaches Modeled

Wisconsin Department
of Natural Resources



Building a PLS model – example for Edgewater, Ohio

2005-2010:
split training data

Build and test models:
predict each fold using
data from the other four

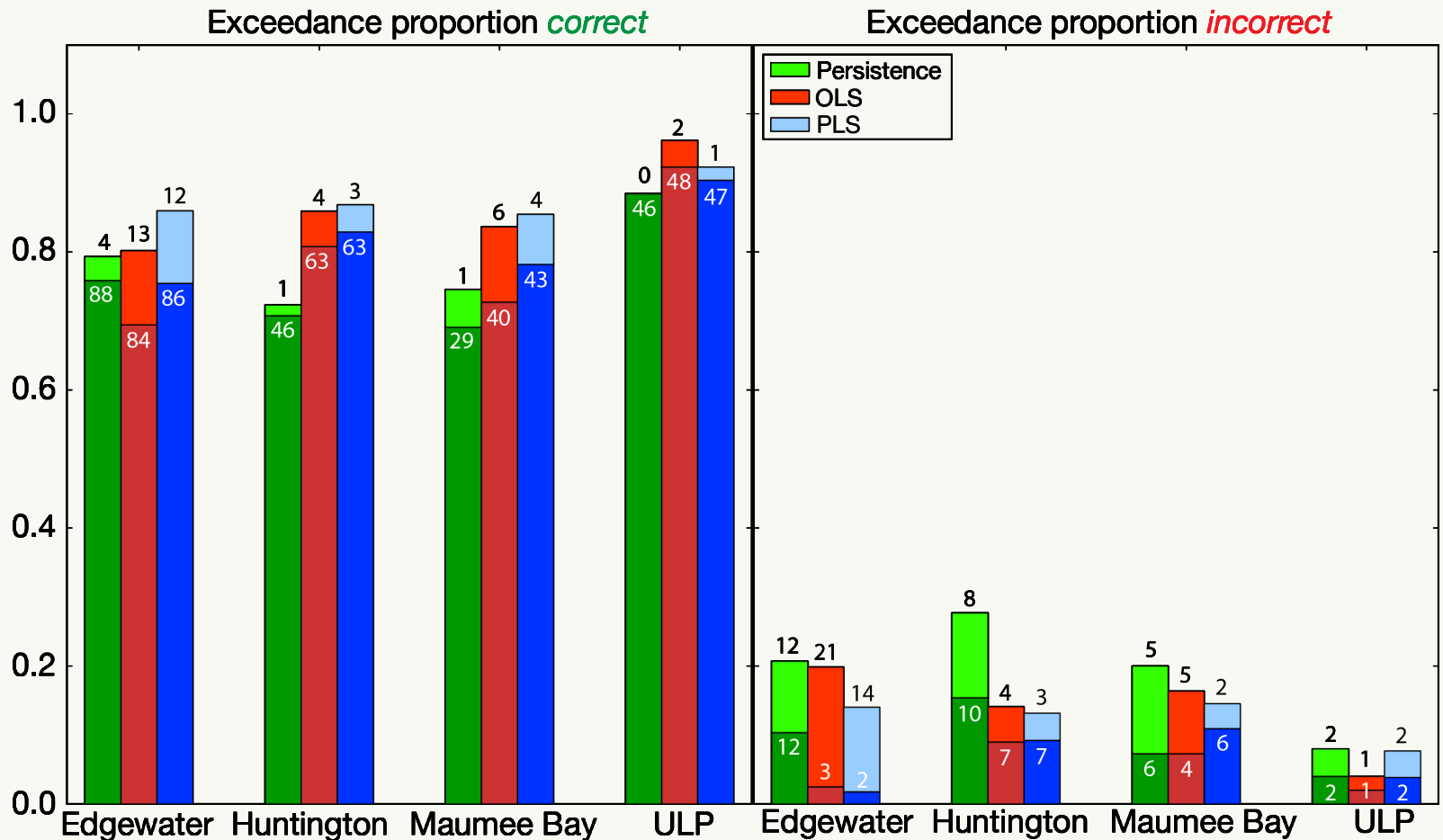
2011:
prediction year

divide the training data
randomly into five equally-
sized “folds”
select a few candidate
specificity limits (tuning)

compare model performance
on the test folds
pick the specificity limit that
had the best performance,
and train a new model over
all five folds

make and record
predictions to manage
beach and provide
data going forward

2010 Model Performance

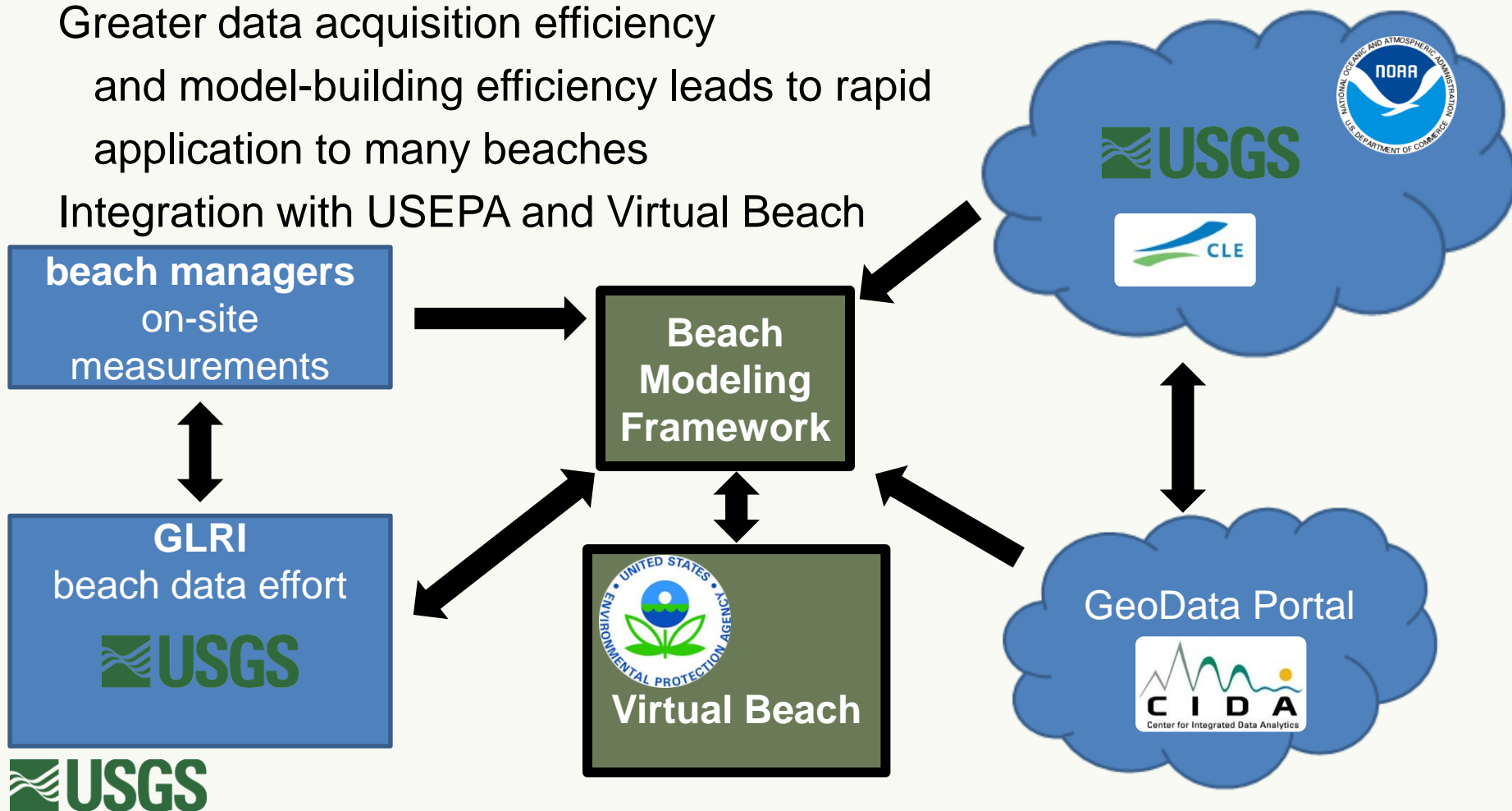


Next Steps

Data acquisition and connectedness

Greater data acquisition efficiency
and model-building efficiency leads to rapid
application to many beaches

Integration with USEPA and Virtual Beach



Next Steps

Virtual Beach

Well-known EPA software for predicting bacterial concentration
PLS regression to be included in version 3 (coming 2012)

The screenshot displays the Virtual Beach 2.2 software interface, specifically the Modeling tab. The interface includes a menu bar (Project, Model, Help) and a tabbed interface with 'Beach Location', 'Data Processing', and 'Modeling'. The 'Modeling' tab is active, showing a 'Variable Selection' section with 'MLR Model' and 'PLS Model' options. The 'PLS Model' is selected, and the 'Number of Observations' is 509. A 'Specificities' input field contains '0.89, 0.91, 0.93' and a 'Run' button. Below this, the 'Model Evaluation Thresholds' section shows a 'Regulatory Standard (Vertical)' of 235. The 'Dependent Variable is:' section has three radio buttons: 'Value', 'Log10 (value)', and 'Loge (value)'. The 'Value' option is selected, and the 'Current US Regulatory Standards' are listed: 'E. coli, Freshwater: 235', 'Enterococci, Freshwater: 104', and 'Enterococci, Saltwater: 61'. A table of model results is displayed, showing specificity, true pos, true neg, false pos, false neg, and total for three specificities: 0.89, 0.91, and 0.93. The row for 0.93 is highlighted. Below the table, a 'Model Summary' section shows the 'Decision Criterion (Horizontal)' as 2.118 and the 'Number of PLS components in the model' as 4. A table of coefficients is also shown, listing variables and their coefficients.

	specificity	true pos	true neg	false pos	false neg	total
0.89	45	388	43	33	509	
0.91	42	391	40	36	509	
0.93	40	400	31	38	509	

Variable	Coefficient
Intercept	-32.8264
year	0.0168
Hop48	0.0165
Hop24	0.0353
Log_turb	0.1573
julan	0.0020
Radar48	0.0292
Radar24	0.1075
wvstck	0.2813

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